

WHAT IS CLAIMED IS:

- 1 1. A method for screening potential catalysts for polymerization performance  
2 comprising:  
3 reacting a potential catalyst with at least a first monomer under polymerization  
4 conditions;  
5 determining the polymerization performance of the catalyst with the at least first  
6 monomer; and  
7 using the determination as a predictor for the polymerization performance of the  
8 catalyst for at least a second monomer;  
9 wherein the first and second monomers are different from each other and the first  
10 monomer is an olefin other than ethylene.
- 1 2. A screening method according to Claim 1 wherein the step of using the  
2 determination as a predictor comprises copolymerizing the first and second monomers  
3 using the catalyst.
- 1 3. A screening method according to Claim 2 comprising copolymerizing the first  
2 and second monomers in commercial quantities using the catalyst.
- 1 4. A screening method according to Claim 1 wherein the step of determining the  
2 polymerization performance comprises measuring at least one property of the reaction  
3 products.
- 1 5. A screening method according to Claim 1 wherein the step of using the  
2 determination as a predictor comprises polymerizing at least the second monomer using  
3 the catalyst.
- 1 6. A screening method according to Claim 1 wherein the step of determining the  
2 polymerization performance comprises measuring the molecular weight of the polymer  
3 formed under the polymerization conditions and using the catalyst.

1 7. A screening method according to Claim 1 wherein the step of determining the  
2 polymerization performance comprises measuring the concentration of the polymer  
3 formed under the polymerization conditions and using the catalyst.

1 8. A screening method according to Claim 1 wherein the step of determining the  
2 polymerization performance comprises measuring the polydispersity index of the  
3 polymer formed under the polymerization conditions and using the catalyst.

1 9. A screening method according to Claim 1 wherein the step of determining the  
2 polymerization performance comprises analyzing the polymer using a high throughput  
3 chromatography technique.

1 10. A screening method according to Claim 9 comprising analyzing the polymer  
2 using size exclusion chromatography.

1 11. A screening method according to Claim 1 comprising reacting the potential  
2 catalyst with a first monomer that is a liquid at room temperature and atmospheric  
3 pressure.

1 12. A screening method according to Claim 1 comprising reacting the potential  
2 catalyst with a monomer selected from the group consisting of 1-octene, 1-hexene, 1-  
3 heptene, 1-nonene, and 1 decene.

1 13. A screening method according to Claim 1, wherein the second monomer is a  
2 gas at room temperature and atmospheric pressure.

1 14. A screening method according to Claim 1, wherein the determination is used  
2 as a predictor for the polymerization performance of the catalyst for a co-polymerization  
3 of two or more monomers which include at least the first monomer.

1 15. A screening method according to Claim 1 wherein the step of reacting the  
2 catalyst with the first monomer comprises reacting the catalyst with 1-octene; and

3 the step of using the determination as a predictor for a second monomer  
4 comprises using the determination as a predictor for a monomer selected from the group  
5 consisting of olefins lower in molecular weight than octene.

1 16. A method of screening potential catalysts for polymerization activity wherein  
2 the polymerization activity of the potential catalysts is determined for at least a first  
3 monomer as a predictor for the polymerization activity of the potential catalysts for at  
4 least a second monomer, the first and second monomers being different from each other  
and the first monomer being an olefin other than ethylene, the method comprising:

6 concurrently reacting an array of at least 8 potential polymerization catalysts that  
7 are different from each other with at least a first monomer under polymerization  
8 conditions; and

9 determining the polymerization performance of each of the potential catalysts  
10 with the at least first monomer.

1 17. A screening method according to Claim 16 further comprising the step of  
2 copolymerizing the first and second monomers using one of the catalysts in the array  
3 based upon the polymerization performance of the catalyst.

1 18. A screening method according to Claim 17 comprising copolymerizing the  
2 first and second monomers in commercial quantities.

1 19. A screening method according to Claim 16 wherein the step of determining  
2 the polymerization performance comprises measuring a characteristic of the reaction  
3 products.

1 20. A screening method according to Claim 16 further comprising the step of  
2 polymerizing the at least second monomer using the catalyst.

1 21. A screening method according to Claim 20 comprising polymerizing the  
2 second monomer in commercial quantities.

1           22. A screening method according to Claim 16 wherein the step of determining  
2 the polymerization performance comprises analyzing the polymer using a high  
3 throughput chromatography technique.

1           23. A screening method according to Claim 22 comprising analyzing the polymer  
2 using size exclusion chromatography.

1           24. A screening method according to Claim 16, wherein the array of potential  
2 catalysts comprises a substrate having wells with each of the at least 8 catalysts residing  
3 in a different well of the substrate.

1           25. A screening method according to Claim 16, wherein the reacting step further  
2 comprises adding other compositions to the wells other than the first or second monomers  
3 or the catalysts.

1           26. A screening method according to Claim 16 comprising dispensing the first  
2 monomer as a liquid into each reaction vessel that contains one of the potential catalysts  
3 prior to the step of reacting the catalyst with the first monomer.

1           27. A screening method according to Claim 16 comprising distributing the first  
2 monomer as a gas to each reaction vessel that contains one of the potential catalysts prior  
3 to the step of reacting the catalyst with the first monomer.

1           28. A screening method according to Claim 16 further comprising:  
2 activating the potential catalysts; and  
3 wherein at least a portion of the at least first monomer is provided to each reaction  
4 vessel prior to activation of the potential catalysts.

1           29. A screening method according to Claim 16, wherein the step of determining  
2 the polymerization performance of the catalysts comprises measuring a property of any  
3 polymer sample made during the reaction step, wherein the property is selected from the  
4 group consisting of molecular weight, polydispersity index, viscosity, concentration,

5 solvent extractables, solubility, melt flow index, glass transition temperature, melting  
6 point, percent crystallinity, density, polymer mass, polymer composition, polymer  
7 structure, polymer architecture, and combinations thereof.

1 30. A screening method according to Claim 16, wherein the determination of  
2 polymerization performance comprises measuring a property of the reaction mixture from  
3 any members of the array, wherein the property is selected from the group consisting of  
4 monomer concentration, monomer conversion, ratio of catalyst to monomer, light  
5 scattering, viscosity, temperature, visual inspection, intrinsic viscosity, polymer  
6 concentration, molecular weight, and combinations thereof.

1 31. A screening method according to Claim 16, wherein the reacting step is  
2 carried out to a predetermined point selected from the group consisting of time, monomer  
3 consumption, heat of reaction, polymer concentration, viscosity, and molecular weight.

1 32. A screening method according to Claim 31 and further comprising quenching  
2 the reaction at the predetermined point.

1 33. A screening method according to Claim 16, wherein the reacting step  
2 comprises concurrently reacting all potential catalysts in the array with the first  
3 monomer.

1 34. A screening method according to Claim 16, wherein the determination is used  
2 as a predictor for the polymerization activity of the potential catalysts for a co-  
3 polymerization of the second monomer with a third monomer.

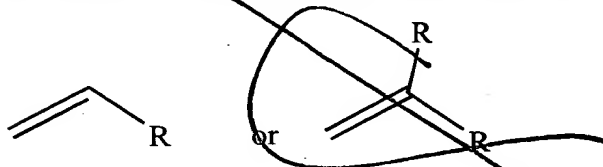
1 35. A screening method according to Claim 34 and further comprising the step of  
2 copolymerizing the second and third monomers.

1 36. A screening method according to Claim 35 comprising copolymerizing the  
2 second and third monomers in commercial quantities.

1 37. A method according to Claim 16 wherein the first monomer is an  $\alpha$ -olefin.

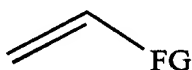
1           38. A method according to Claim 37 wherein the first monomer is selected from  
2 the group consisting of 1-octene, 1-hexene, 1-heptene, 1-nonene, and 1 decene.

3  
4           39. A screening method according to Claim 14, wherein the at least first  
5 monomer is an  $\alpha$ -olefin represented by either formula:



7 wherein each R is independently selected from the group consisting of halogen, alkyl,  
8 substituted alkyl, aryl, substituted aryl, heteroalkyl, cycloalkyl, substituted cycloalkyl,  
9 heterocycloalkyl, substituted heterocycloalkyl, heteroaryl, substituted heteroaryl, alkoxy,  
10 silyl, boryl, phosphino, amino, thio, seleno and combinations thereof.

1           40. A screening method according to Claim 16 wherein at least the first monomer  
2 is represented by the formula:



4 wherein FG is a halogen or a functional group that contains at least one heteroatom.

5  
6           41. A screening method according to Claim 16 comprising:  
7 measuring the polymerization activity of each of the potential catalysts with the at  
8 least first monomer; and

9 predicting the polymerization activity of each of the potential catalysts for at least  
10 a second monomer, wherein the first and second monomers are chemically different from  
each other and the first monomer is an olefin other than ethylene.

1           42. A screening method for high throughput screening of potential catalysts for  
2 polymerization activity for at least a second monomer, comprising:

3 concurrently reacting a plurality of at least 8 potential catalysts arrayed on a  
4 substrate with a first monomer; and

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Contd.

determining a property of any polymer sample or polymerization mixture made during the reaction step at a rate of one hour or less per potential catalyst.

1 43. A screening method according to Claim 42 comprising:  
2 concurrently reacting at least 24 potential catalysts; and  
3 determining properties at a rate of about 20 minutes or less per potential catalyst.

1 44. A screening method according to Claim 42 wherein the step of determining  
2 the polymerization performance comprises measuring a characteristic of the reaction  
3 products.

1 45. A screening method according to Claim 42 wherein the step of determining a  
2 property comprises measuring the concentration of the polymer formed using the catalyst.

1 46. A screening method according to Claim 42 wherein the step of determining a  
2 property comprises measuring the polydispersity index of the polymer formed using the  
3 catalyst.

1 47. A screening method according to Claim 42 wherein the step of determining a  
2 property comprises analyzing the polymer using a high throughput chromatography  
3 technique.

1 48. A screening method according to Claim 47 comprising analyzing the polymer  
2 using size exclusion chromatography.

1 49. A screening method according to Claim 42, wherein the step of determining a  
2 property comprises measuring a property of any polymer sample made during the  
3 reaction step, wherein the property is selected from the group consisting of molecular  
4 weight, polydispersity index, viscosity, concentration, solvent extractables, solubility,  
5 melt flow index, glass transition temperature, melting point, percent crystallinity, density,  
6 polymer mass, polymer composition, polymer structure, polymer architecture, and  
7 combinations thereof.

1           50. A screening method according to Claim 42, wherein the step of determining a  
2 property comprises measuring a property of the polymerization reaction mixture from  
3 any members of the array, wherein the property is selected from the group consisting of  
4 monomer concentration, monomer conversion, ratio of catalyst to monomer, light  
5 scattering, viscosity, temperature, visual inspection, intrinsic viscosity, polymer  
6 concentration, molecular weight, and combinations thereof.

1           51. A screening method according to Claim 42, wherein the concurrent reactions  
2 are carried out to a predetermined point selected from the group consisting of time,  
3 monomer consumption, heat of reaction, polymer concentration, viscosity, and molecular  
4 weight.

1           52. A screening method according to Claim 51 and further comprising  
2 concurrently quenching the reaction at the predetermined point.

1           53. A screening method according to Claim 42, wherein the determination is used  
2 as a predictor for the polymerization activity of the potential catalysts for a co-  
3 polymerization of the second monomer with at least a third monomer.

1           54. A screening method according to Claim 53 and further comprising the step of  
2 copolymerizing the at least second and third monomers.

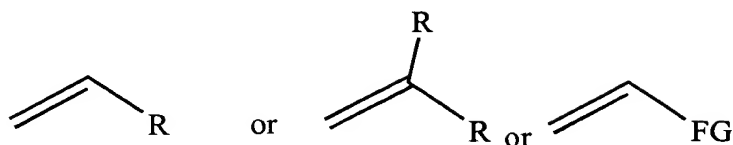
1           55. A screening method according to Claim 54 comprising copolymerizing the at  
2 least second and third monomers in commercial quantities.

1           56. A method according to Claim 42 wherein the first monomer is an olefin other  
2 than ethylene.

1           57. A method according to Claim 42 wherein the first monomer is 1-octene, 1-  
2 hexene, 1-heptene, 1-nonene, and 1 decene.

1           58. A screening method according to Claim 41, wherein the first monomer is  
2 represented by a formula selected from the group consisting of:





4 wherein each R is independently selected from the group consisting of halogen, alkyl,  
5 substituted alkyl, aryl, substituted aryl, heteroalkyl, cycloalkyl, substituted cycloalkyl,  
6 heterocycloalkyl, substituted heterocycloalkyl, heteroaryl, substituted heteroaryl, alkoxy,  
7 sityl, boryl, phosphino, amino, thio, seleno and combinations thereof; and FG is halogen  
8 or a functional group that contains at least one heteroatom.

1 59. A method for high throughput screening of potential catalysts for  
2 polymerization activity for at least a second monomer, comprising:  
3 combining a plurality of catalysts with an array of portions of a first monomer,  
4 with the number of portions of monomers being greater than the number of catalysts, and  
5 with no more than one catalyst in each of the monomer portions;  
6 concurrently initiating a polymerization reaction in each of the monomer portions;  
7 concurrently quenching the polymerization reaction in each of the monomer  
8 portions; and  
9 sampling the portions at a rate of between about 30 seconds and eight minutes per  
10 sample.

1 60. A screening method according to Claim 59 comprising combining the  
2 plurality of catalyst with 96 portions of the first monomer.

1 61. A screening method according to Claim 59, wherein the step of sampling the  
2 portions comprises determining a property of the sample selected from the group  
3 consisting of polymer properties and polymerization mixture properties.

1 62. A screening method according to Claim 59 and further comprising the step of  
2 combining ligands and metal precursors to form the catalysts prior to the step of  
3 combining the catalysts with the monomer portions.

1 63. A screening method according to Claim 62 further comprising combining the  
2 catalysts with one or more activators.

1 64. A catalyst library comprising:  
2 a plurality of compounds;  
3 a benchmark quality of polymerization of a particular olefin; and  
4 the information as to whether each compound falls above or below the olefin-  
5 polymerization benchmark.

01 65. A catalyst library comprising:  
02 a plurality of compounds;  
03 a benchmark quality of the polymerization of 1-octene; and  
04 the information as to whether each compound falls above or below the octene  
05 polymerization benchmark.

01 66. A catalyst library according to Claim 65 wherein the benchmark quality is  
02 selected from the group consisting of: molecular weight, polymerization rate, viscosity,  
03 concentration, solvent extractables, solubility, melt flow index, glass transition  
04 temperature, melting point, percent crystallinity, density, polymer mass, polymer  
5 composition, polymer structure, polymer architecture, monomer concentration, monomer  
6 conversion, ratio of catalyst to monomer, light scattering, viscosity, temperature, visual  
7 inspection, intrinsic viscosity, polymer concentration, molecular weight, and  
8 combinations thereof.

1 67. A method of producing a benchmark library for the polymerization of olefins  
2 comprising screening a plurality of catalysts against the benchmark at a rate of between  
3 about 30 seconds and 20 minutes per catalyst.

1 68. The method of claim 67, wherein the rate is between about 30 seconds and 10  
2 minutes.

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1 69. The method of claim 68 wherein the rate is between about 30 seconds and  
2 8minutes.

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